Succinic acid, 2,3-dichlorophenyl 1,1,1-trifluoroprop-2-yl ester

Inchi: InChI=1S/C13H11Cl2F3O4/c1-7(13(16,17)18)21-10(19)5-6-11(20)22-9-4-2-3-8(14)12(9)1

InchiKey: MTQAJSNCBBKNEB-UHFFFAOYSA-N

Formula: C13H11Cl2F3O4

SMILES: CC(OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl)C(F)(F)F

Mol. weight [g/mol]: 359.12

Physical Properties

Property code	Value	Unit	Source
gf	-924.00	kJ/mol	Joback Method
hf	-1221.50	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.173		Crippen Method
mcvol	214.940	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	755.06	K	Joback Method
tc	960.89	K	Joback Method
tf	481.08	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.96	J/mol×K	755.06	Joback Method
cpg	572.56	J/mol×K	789.36	Joback Method
cpg	582.32	J/mol×K	823.67	Joback Method
cpg	591.27	J/mol×K	857.97	Joback Method
cpg	599.43	J/mol×K	892.28	Joback Method
cpg	606.83	J/mol×K	926.58	Joback Method
cpg	613.48	J/mol×K	960.89	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume